Jin-Long Yang

List of Publications by Year in Descending Order

503 papers	28,709 citations	89 h-index	150 g-index
533 ext. papers	33,296 ext. citations	7.9 avg, IF	7.63 L-index

#	Paper	IF	Citations
503	In Situ Low-Temperature Growth and Superior Luminescent Property of Well-Aligned, High-Quality Cubic CsPbBr Micrometer-Scale Single Crystal Arrays on Transparent Conductive Substrates.. *Journal of Physical Chemistry Letters*, **2022**, 1114-1122	6.4	0
502	CN/ScCCl Weak van der Waals Heterostructure: A Promising Visible-Light-Driven -Scheme Water Splitting Photocatalyst with Interface Ultrafast Carrier Recombination.. *Journal of Physical Chemistry Letters*, **2022**, 1473-1479	6.4	4
501	The Journal of Physical Chemistry C Virtual Special Issue on Energy and Catalysis in China *Journal of Physical Chemistry C*, **2022**, 126, 2301-2306	3.8	
500	Mixed magnetic edge states in graphene quantum dots. *Multifunctional Materials*, **2022**, 5, 014001	5.2	
499	Computational characterization of nanosystems. *Chinese Journal of Chemical Physics*, **2022**, 35, 1-15	0.9	
498	Schottky and Ohmic Contacts at Tellurene/2D Metal Interfaces. *ACS Applied Electronic Materials*, **2022**, 4, 1082-1088	4	2
497	Theoretical design of two-dimensional visible light-driven photocatalysts for overall water splitting. *Chemical Physics Reviews*, **2022**, 3, 011310	4.4	1
496	Single-molecule field effect and conductance switching driven by electric field and proton transfer.. *Science Advances*, **2022**, 8, eabm3541	14.3	5
495	High-Throughput Computational Screening for Bipolar Magnetic Semiconductors.. *Research*, **2022**, 2022, 9857631	7.8	0
494	Promoting Water Activation by Photogenerated Holes in Monolayer CN.. *Journal of Physical Chemistry Letters*, **2022**, 3332-3337	6.4	0
493	Molecular Design of Two-Dimensional Covalent Heptazine Frameworks for Photocatalytic Overall Water Splitting under Visible Light.. *Journal of Physical Chemistry Letters*, **2022**, 13, 3949-3956	6.4	1
492	High-performance photocatalytic nonoxidative conversion of methane to ethane and hydrogen by heteroatoms-engineered TiO.. *Nature Communications*, **2022**, 13, 2806	17.4	7
491	KSSOLV 2.0: An efficient MATLAB toolbox for solving the Kohn-Sham equations with plane-wave basis set. *Computer Physics Communications*, **2022**, 108424	4.2	2
490	Understanding Single-Atom Catalysis in View of Theory.. *Jacs Au*, **2021**, 1, 2130-2145		16
489	Two-dimensional bipolar magnetic semiconductors with high Curie-temperature and electrically controllable spin polarization realized in exfoliated Cr(pyrazine)2 monolayers. *Science China Chemistry*, **2021**, 64, 2212	7.9	4
488	Designing Two-Dimensional Versatile Room-Temperature Ferromagnets via Assembling Large-Scale Magnetic Quantum Dots. *Nano Letters*, **2021**, 21, 9816-9823	11.5	5
487	Improving the Activity of Electrocatalysts toward the Hydrogen Evolution Reaction, the Oxygen Evolution Reaction, and the Oxygen Reduction Reaction via Modification of Metal and Ligand of Conductive Two-Dimensional Metal-Organic Frameworks. *Journal of Physical Chemistry Letters*, **2021**, 12, 11652-11658	6.4	6

486	High Curie Temperature and Intrinsic Ferromagnetic Half-Metallicity in MnX (X = S, Se, Te) Nanosheets. *Journal of Physical Chemistry Letters*, **2021**, 11790-11794	6.4	2
485	First-Principles Calculations of Room-Temperature Antiferromagnetism in Crystalline Transition-Metal Borate Nanosheets: Implications for Spintronics Applications. *ACS Applied Nano Materials*, **2021**, 4, 10877-10885	5.6	1
484	Nodal-loop half metallicity in a two-dimensional FeN pentagon crystal with room-temperature ferromagnetism. *Nanoscale*, **2021**, 13, 19493-19499	7.7	3
483	Two-Dimensional Giant Tunable Rashba Semiconductors with Two-Atom-Thick Buckled Honeycomb Structure. *Nano Letters*, **2021**, 21, 740-746	11.5	15
482	Capturing the Electron-Phonon Renormalization in Molecules from First-Principles. *Journal of Physical Chemistry A*, **2021**, 125, 2682-2689	2.8	1
481	Assessment of the Mass Factor for the Electron□Phonon Coupling in Solids. *Journal of Physical Chemistry C*, **2021**, 125, 6479-6485	3.8	1
480	A single-molecule electrical approach for amino acid detection and chirality recognition. *Science Advances*, **2021**, 7,	14.3	9
479	Orbital Design of Two-Dimensional Transition-Metal Peroxide Kagome Crystals with Anionogenic Dirac Half-Metallicity. *Journal of Physical Chemistry Letters*, **2021**, 12, 3528-3534	6.4	1
478	2D Heterostructured Nanofluidic Channels for Enhanced Desalination Performance of Graphene Oxide Membranes. *ACS Nano*, **2021**, 15, 7586-7595	16.7	25
477	Efficient Direct Band Gap Photovoltaic Material Predicted Via Doping Double Perovskites Cs2AgBiX6 (X = Cl, Br). *Journal of Physical Chemistry C*, **2021**, 125, 10868-10875	3.8	10
476	Generated High-Valent Iron Single-Atom Catalyst for Efficient Oxygen Evolution. *Nano Letters*, **2021**, 21, 4795-4801	11.5	17
475	Hybrid MPI and OpenMP parallel implementation of large-scale linear-response time-dependent density functional theory with plane-wave basis set. *Electronic Structure*, **2021**, 3, 024004	2.6	0
474	An efficient adaptive variational quantum solver of the Schr□inger equation based on reduced density matrices. *Journal of Chemical Physics*, **2021**, 154, 244112	3.9	3
473	Efficient interlayer charge release for high-performance layered thermoelectrics. *National Science Review*, **2021**, 8, nwaa085	10.8	9
472	High performance computing of DGDFT for tens of thousands of atoms using millions of cores on Sunway TaihuLight. *Science Bulletin*, **2021**, 66, 111-119	10.6	5
471	Efficient parallel linear scaling method to get the response density matrix in all-electron real-space density-functional perturbation theory. *Computer Physics Communications*, **2021**, 258, 107613	4.2	2
470	Formation of Plasmonic Polarons in Highly Electron-Doped Anatase TiO. *Nano Letters*, **2021**, 21, 430-436	11.5	3
469	Single Mo1(W1, Re1) atoms anchored in pyrrolic-N3 doped graphene as efficient electrocatalysts for the nitrogen reduction reaction. *Journal of Materials Chemistry A*, **2021**, 9, 6547-6554	13	11

468	Strain-Stabilized Metastable Face-Centered Tetragonal Gold Overlayer for Efficient CO Electroreduction. *Nano Letters*, **2021**, 21, 1003-1010	11.5	15
467	Doping dependence of electronic structure of infinite-layer NdNiO2. *Physical Review B*, **2021**, 103,	3.3	10
466	CrSbS monolayer: a potential phase transition ferromagnetic semiconductor. *Nanoscale*, **2021**, 13, 14067-14072	7.1	21
465	Determining structural and chemical heterogeneities of surface species at the single-bond limit. *Science*, **2021**, 371, 818-822	33.3	32
464	Probing intramolecular vibronic coupling through vibronic-state imaging. *Nature Communications*, **2021**, 12, 1280	17.4	15
463	Tunable Rashba Spin Splitting in Two-Dimensional Polar Perovskites. *Journal of Physical Chemistry Letters*, **2021**, 12, 1932-1939	6.4	4
462	Raman Detection of Bond Breaking and Making of a Chemisorbed Up-Standing Single Molecule at Single-Bond Level. *Journal of Physical Chemistry Letters*, **2021**, 12, 1961-1968	6.4	8
461	Two-level iterative solver for linear response time-dependent density functional theory with plane wave basis set. *Journal of Chemical Physics*, **2021**, 154, 064101	3.9	3
460	Thickness Dependent Magnetic Transition in Few Layer 1T Phase CrTe. *Journal of Physical Chemistry Letters*, **2021**, 12, 6847-6851	6.4	6
459	Electric-Field Tunable Magnetism in van der Waals Bilayers with A-Type Antiferromagnetic Order: Unipolar versus Bipolar Magnetic Semiconductor. *Nano Letters*, **2021**, 21, 7050-7055	11.5	6
458	Realizing Effective Cubic-Scaling Coulomb Hole Plus Screened Exchange Approximation in Periodic Systems via Interpolative Separable Density Fitting with a Plane-Wave Basis Set. *Journal of Physical Chemistry A*, **2021**, 125, 7545-7557	2.8	4
457	An efficient nanocluster catalyst for Sonogashira reaction. *Journal of Catalysis*, **2021**, 401, 206-213	7.3	3
456	Unveiling the full reaction path of the Suzuki-Miyaura cross-coupling in a single-molecule junction. *Nature Nanotechnology*, **2021**, 16, 1214-1223	28.7	13
455	Equation-of-Motion Theory to Calculate Accurate Band Structures with a Quantum Computer. *Journal of Physical Chemistry Letters*, **2021**, 12, 8833-8840	6.4	2
454	An efficient implementation of spin-orbit coupling within the framework of semiempirical orthogonalization-corrected methods for ultrafast intersystem crossing dynamics. *Physical Chemistry Chemical Physics*, **2021**, 23, 22313-22323	3.6	2
453	A rationally designed two-dimensional MoSe/TiCO heterojunction for photocatalytic overall water splitting: simultaneously suppressing electron-hole recombination and photocorrosion. *Chemical Science*, **2021**, 12, 2863-2869	9.4	26
452	Spin-Orbit Coupling in 2D Semiconductors: A Theoretical Perspective.. *Journal of Physical Chemistry Letters*, **2021**, 12, 12256-12268	6.4	6
451	Low-Rank Approximations Accelerated Plane-Wave Hybrid Functional Calculations with k-Point Sampling.. *Journal of Chemical Theory and Computation*, **2021**,	6.4	6

450	Designing Direct Z-Scheme Heterojunctions Enabled by Edge-Modified Phosphorene Nanoribbons for Photocatalytic Overall Water Splitting.. *Journal of Physical Chemistry Letters*, **2021**, 1-11	6.4	5
449	Precise Spin Manipulation of Single Molecule Positioning on Graphene by Coordination Chemistry. *Journal of Physical Chemistry Letters*, **2020**, 11, 9819-9827	6.4	3
448	Photogenerated-Carrier Separation and Transfer in Two-Dimensional Janus Transition Metal Dichalcogenides and Graphene van der Waals Sandwich Heterojunction Photovoltaic Cells. *Journal of Physical Chemistry Letters*, **2020**, 11, 4070-4079	6.4	23
447	Electronic and magnetic structure of infinite-layer NdNiO2: trace of antiferromagnetic metal. *Npj Quantum Materials*, **2020**, 5,	5	38
446	Tunable n-type and p-type doping of two-dimensional layered PdSevia organic molecular adsorption. *Physical Chemistry Chemical Physics*, **2020**, 22, 12973-12979	3.6	5
445	Two-Dimensional Multifunctional Metal-Organic Frameworks with Simultaneous Ferro-/Ferrimagnetism and Vertical Ferroelectricity. *Journal of Physical Chemistry Letters*, **2020**, 11, 4193-4197	6.4	14
444	Direct bandgap engineering with local biaxial strain in few-layer MoS2 bubbles. *Nano Research*, **2020**, 13, 2072-2078	10	10
443	Interpolative Separable Density Fitting Decomposition for Accelerating Hartree-Fock Exchange Calculations within Numerical Atomic Orbitals. *Journal of Physical Chemistry A*, **2020**, 124, 5664-5674	2.8	8
442	Halogen modified two-dimensional covalent triazine frameworks as visible-light driven photocatalysts for overall water splitting. *Science China Chemistry*, **2020**, 63, 1134-1141	7.9	17
441	Structural Oscillation Revealed in Gold Nanoparticles. *Journal of the American Chemical Society*, **2020**, 142, 12140-12145	16.4	27
440	The Moving-Grid Effect in the Harmonic Vibrational Frequency Calculations with Numeric Atom-Centered Orbitals. *Journal of Physical Chemistry A*, **2020**, 124, 2897-2906	2.8	2
439	The dynamic parallel distribution algorithm for hybrid density-functional calculations in HONPAS package. *Computer Physics Communications*, **2020**, 254, 107204	4.2	2
438	Two-dimensional CaN as a one-dimensional electride [CaN]2e with ultrahigh conductance. *Nanoscale*, **2020**, 12, 5578-5586	7.7	1
437	Tunable Rashba spin splitting in Janus transition-metal dichalcogenide monolayers charge doping.. *RSC Advances*, **2020**, 10, 6388-6394	3.7	25
436	Creation of the Dirac Nodal Line by Extrinsic Symmetry Engineering. *Nano Letters*, **2020**, 20, 2157-2162	11.5	1
435	A Simple Molecular Design Strategy for Two-Dimensional Covalent Organic Framework Capable of Visible-Light-Driven Water Splitting. *Journal of the American Chemical Society*, **2020**, 142, 4508-4516	16.4	92
434	Atomic-Level Construction of Tensile-Strained PdFe Alloy Surface toward Highly Efficient Oxygen Reduction Electrocatalysis. *Nano Letters*, **2020**, 20, 1403-1409	11.5	50
433	Low-cost alternatives to the Bethe-Salpeter equation: Towards simple hybrid functionals for excitonic effects in solids. *Physical Review Research*, **2020**, 2,	3.9	18

432	Parallel Implementation of Large-Scale Linear Scaling Density Functional Theory Calculations With Numerical Atomic Orbitals in HONPAS. *Frontiers in Chemistry*, **2020**, 8, 589910	5	0
431	Implementation of Laplace Transformed MP2 for Periodic Systems With Numerical Atomic Orbitals. *Frontiers in Chemistry*, **2020**, 8, 589992	5	3
430	Steric Hindrance Effect in High-Temperature Reactions. *CCS Chemistry*, **2020**, 2, 460-467	7.2	13
429	Module Replacement of Gold Nanoparticles by a Pseudo-AGR Process. *Acta Chimica Sinica*, **2020**, 78, 407	3.3	9
428	Are pyridinium ylides radicals?. *Chemical Communications*, **2020**, 56, 11287-11290	5.8	2
427	Molecular molds for regularizing Kondo states at atom/metal interfaces. *Nature Communications*, **2020**, 11, 2566	17.4	10
426	Low-threshold amplification of spontaneous emission from AgInS2 quantum dots. *Journal of Materials Chemistry C*, **2020**, 8, 8515-8520	7.1	3
425	Oscillation of Work Function during Reducible Metal Oxide Catalysis and Correlation with the Activity Property. *ChemCatChem*, **2020**, 12, 85-89	5.2	1
424	Accelerating Excitation Energy Computation in Molecules and Solids within Linear-Response Time-Dependent Density Functional Theory via Interpolative Separable Density Fitting Decomposition. *Journal of Chemical Theory and Computation*, **2020**, 16, 964-973	6.4	10
423	Interfacial Hydrogen-Bonding Dynamics in Surface-Facilitated Dehydrogenation of Water on TiO(110). *Journal of the American Chemical Society*, **2020**, 142, 826-834	16.4	14
422	Atomic-level insights into strain effect on p-nitrophenol reduction via Au@Pd core–shell nanocubes as an ideal platform. *Journal of Catalysis*, **2020**, 381, 427-433	7.3	18
421	Simulating Periodic Systems on a Quantum Computer Using Molecular Orbitals. *Journal of Chemical Theory and Computation*, **2020**, 16, 6904-6914	6.4	3
420	Machine Learning K-Means Clustering Algorithm for Interpolative Separable Density Fitting to Accelerate Hybrid Functional Calculations with Numerical Atomic Orbitals. *Journal of Physical Chemistry A*, **2020**, 124, 10066-10074	2.8	9
419	Highly efficient heterojunction solar cells enabled by edge-modified tellurene nanoribbons. *Physical Chemistry Chemical Physics*, **2020**, 22, 28414-28422	3.6	4
418	Sub-nanometre resolution in single-molecule photoluminescence imaging. *Nature Photonics*, **2020**, 14, 693-699	33.9	69
417	Me-graphene: a graphene allotrope with near zero Poisson's ratio, sizeable band gap, and high carrier mobility. *Nanoscale*, **2020**, 12, 19359-19366	7.7	13
416	Realizing CsPbBr Light-Emitting Diode Arrays Based on PDMS Template Confined Solution Growth of Single-Crystalline Perovskite. *Journal of Physical Chemistry Letters*, **2020**, 11, 8275-8282	6.4	10
415	Ion-molecule reactions catalyzed by a single gold atom. *Chemical Science*, **2020**, 11, 8502-8505	9.4	1

414	Proposed mechanical method for switching the spin transport channel in two-dimensional magnetic metal-magnetic semiconductor van der Waals contacts. *Nanoscale Horizons*, **2020**, 5, 1496-1499	10.8	2
413	Modulating oxygen coverage of TiCT MXenes to boost catalytic activity for HCOOH dehydrogenation. *Nature Communications*, **2020**, 11, 4251	17.4	35
412	Identifying the Molecular Orientation and Clusters in the Liquid-Vapor Interface of 1-Propanol by Time-Delayed Mass Spectrometry. *Journal of Physical Chemistry Letters*, **2020**, 11, 7510-7516	6.4	4
411	One-Dimensional Magnetic Order Stabilized in Edge-Reconstructed MoS Nanoribbon via Bias Voltage. *Journal of Physical Chemistry Letters*, **2020**, 11, 7531-7535	6.4	6
410	The static parallel distribution algorithms for hybrid density-functional calculations in HONPAS package. *International Journal of High Performance Computing Applications*, **2020**, 34, 159-168	1.8	2
409	Large-Spin-Gap Nodal-Line Half-Metal and High-Temperature Ferromagnetic Semiconductor in Cr2X3 (X=O,S,Se) Monolayers. *Advanced Electronic Materials*, **2020**, 6, 1900490	6.4	15
408	Descriptor-Based Design Principle for Two-Dimensional Single-Atom Catalysts: Carbon Dioxide Electroreduction. *Journal of Physical Chemistry Letters*, **2020**, 11, 3481-3487	6.4	34
407	The Contacts of the Monolayer Semiconductor C2N with 2D Metal Electrodes. *Advanced Theory and Simulations*, **2019**, 2, 1800161	3.5	8
406	Unconventional p-d Hybridization Interaction in PtGa Ultrathin Nanowires Boosts Oxygen Reduction Electrocatalysis. *Journal of the American Chemical Society*, **2019**, 141, 18083-18090	16.4	107
405	Atomically dispersed iron hydroxide anchored on Pt for preferential oxidation of CO in H. *Nature*, **2019**, 565, 631-635	50.4	260
404	Ion Conductivity Enhancement in Anti-Spinel Li3OBr with Intrinsic Vacancies. *Advanced Theory and Simulations*, **2019**, 2, 1800138	3.5	9
403	Fcc versus Non-fcc Structural Isomerism of Gold Nanoparticles with Kernel Atom Packing Dependent Photoluminescence. *Angewandte Chemie*, **2019**, 131, 4558-4562	3.6	9
402	Fcc versus Non-fcc Structural Isomerism of Gold Nanoparticles with Kernel Atom Packing Dependent Photoluminescence. *Angewandte Chemie - International Edition*, **2019**, 58, 4510-4514	16.4	36
401	Proposal of a stable B3S nanosheet as an efficient hydrogen evolution catalyst. *Journal of Materials Chemistry A*, **2019**, 7, 3752-3756	13	22
400	Transition-Metal Diboride: A New Family of Two-Dimensional Materials Designed for Selective CO2 Electroreduction. *Journal of Physical Chemistry C*, **2019**, 123, 16294-16299	3.8	25
399	Spin-Crossover and Coherent Transport Behaviors of a Six-Coordinate Iron(II) Complex with a N4O2 Donor Set. *Journal of Physical Chemistry C*, **2019**, 123, 16366-16372	3.8	9
398	Electrically Driven Single-Photon Superradiance from Molecular Chains in a Plasmonic Nanocavity. *Physical Review Letters*, **2019**, 122, 233901	7.4	32
397	Toward Room-Temperature Magnetic Semiconductors in Two-Dimensional Ferrimagnetic Organometallic Lattices. *Journal of Physical Chemistry Letters*, **2019**, 10, 2439-2444	6.4	21

396	Room-temperature magnetism and tunable energy gaps in edge-passivated zigzag graphene quantum dots. *Npj 2D Materials and Applications*, **2019**, 3,	8.8	19
395	Room temperature electrofreezing of water yields a missing dense ice phase in the phase diagram. *Nature Communications*, **2019**, 10, 1925	17.4	13
394	Single Mo1(Cr1) Atom on Nitrogen-Doped Graphene Enables Highly Selective Electroreduction of Nitrogen into Ammonia. *ACS Catalysis*, **2019**, 9, 3419-3425	13.1	170
393	Highly-efficient heterojunction solar cells based on two-dimensional tellurene and transition metal dichalcogenides. *Journal of Materials Chemistry A*, **2019**, 7, 7430-7436	13	54
392	Electronic and magnetic properties of CoPc and FePc molecules on graphene: the substrate, defect, and hydrogen adsorption effects. *Physical Chemistry Chemical Physics*, **2019**, 21, 5424-5434	3.6	10
391	Room-Temperature Ferromagnetism in Transition Metal Embedded Borophene Nanosheets. *Journal of Physical Chemistry Letters*, **2019**, 10, 4417-4421	6.4	20
390	Significantly Enhanced Charge Separation in Rippled Monolayer Graphitic C3N4. *ChemCatChem*, **2019**, 11, 6252-6257	5.2	8
389	Computational Design of One-Dimensional Ferromagnetic Semiconductors in Transition Metal Embedded Stannaspherene Nanowires. *Chinese Journal of Chemistry*, **2019**, 37, 1021-1024	4.9	3
388	Dynamic oxygen adsorption on single-atomic Ruthenium catalyst with high performance for acidic oxygen evolution reaction. *Nature Communications*, **2019**, 10, 4849	17.4	194
387	Tunable Schottky and Ohmic contacts in graphene and tellurene van der Waals heterostructures. *Physical Chemistry Chemical Physics*, **2019**, 21, 23611-23619	3.6	14
386	Spin Selection Rule in Single-Site Catalysis of Molecular Oxygen Adsorption on Transition-Metal Phthalocyanines. *Journal of Physical Chemistry C*, **2019**, 123, 28158-28167	3.8	1
385	Tuning Electronic Structure and Lattice Diffusion Barrier of Ternary PtInNi for Both Improved Activity and Stability Properties in Oxygen Reduction Electrocatalysis. *ACS Catalysis*, **2019**, 9, 11431-11437	13.1	21
384	Quasi PdNi single-atom surface alloy catalyst enables hydrogenation of nitriles to secondary amines. *Nature Communications*, **2019**, 10, 4998	17.4	48
383	Visually constructing the chemical structure of a single molecule by scanning Raman picoscopy. *National Science Review*, **2019**, 6, 1169-1175	10.8	51
382	Revealing Charge- and Temperature-Dependent Movement Dynamics and Mechanism of Individual Molecular Machines. *Small Methods*, **2019**, 3, 1900464	12.8	12
381	The Synthesis of Chiral Ag4Pd2(SR)8 by Nonreplaced Galvanic Reaction. *Particle and Particle Systems Characterization*, **2019**, 36, 1900003	3.1	10
380	Control of highly anisotropic electrical conductance of tellurene by strain-engineering. *Nanoscale*, **2019**, 11, 21775-21781	7.7	8
379	Spin-flip excitations induced by dehydrogenation in a magnetic single-molecule junction. *Journal of Chemical Physics*, **2019**, 151, 224704	3.9	4

378	Realizing Two-Dimensional Magnetic Semiconductors with Enhanced Curie Temperature by Antiaromatic Ring Based Organometallic Frameworks. *Journal of the American Chemical Society*, **2019**, 141, 109-112	16.4	46
377	Identification of single-atom active sites in carbon-based cobalt catalysts during electrocatalytic hydrogen evolution. *Nature Catalysis*, **2019**, 2, 134-141	36.5	409
376	Construction of direct Z-Scheme photocatalysts for overall water splitting using two-dimensional van der waals heterojunctions of metal dichalcogenides. *Journal of Computational Chemistry*, **2019**, 40, 980-987	3.5	34
375	Competitive Transient Electrostatic Adsorption for In Situ Regeneration of Poisoned Catalyst. *ChemCatChem*, **2019**, 11, 1179-1184	5.2	0
374	Azide Passivation of Black Phosphorus Nanosheets: Covalent Functionalization Affords Ambient Stability Enhancement. *Angewandte Chemie - International Edition*, **2019**, 58, 1479-1483	16.4	79
373	Kernel Tuning and Nonuniform Influence on Optical and Electrochemical Gaps of Bimetal Nanoclusters. *Journal of the American Chemical Society*, **2018**, 140, 3487-3490	16.4	61
372	Direct observation of single-molecule hydrogen-bond dynamics with single-bond resolution. *Nature Communications*, **2018**, 9, 807	17.4	56
371	Atomistic Simulations of Graphene Growth: From Kinetics to Mechanism. *Accounts of Chemical Research*, **2018**, 51, 728-735	24.3	20
370	Water Confined in Nanocapillaries: Two-Dimensional Bilayer Squarelike Ice and Associated Solid□Liquid□Solid Transition. *Journal of Physical Chemistry C*, **2018**, 122, 6704-6712	3.8	21
369	Pressure-induced organic topological nodal-line semimetal in the three-dimensional molecular crystal Pd(dddt)2. *Physical Review B*, **2018**, 97,	3.3	16
368	Coronoid nanographene C216 as hydrogen purification membrane: A density functional theory study. *Carbon*, **2018**, 135, 112-117	10.4	3
367	Light-Induced Type-II Band Inversion and Quantum Anomalous Hall State in Monolayer FeSe. *Physical Review Letters*, **2018**, 120, 156406	7.4	18
366	A short review of nanographenes: structures, properties and applications. *Molecular Physics*, **2018**, 116, 987-1002	1.7	8
365	First-Principles Study on Layered CN-Metal Interfaces. *Langmuir*, **2018**, 34, 2647-2653	4	10
364	Is the kernel-staples match a key-lock match?. *Chemical Science*, **2018**, 9, 2437-2442	9.4	37
363	Surface alloy engineering in 2D trigonal lattice: giant Rashba spin splitting and two large topological gaps. *New Journal of Physics*, **2018**, 20, 023041	2.9	6
362	A high performance catalyst for methane conversion to methanol: graphene supported single atom Co. *Chemical Communications*, **2018**, 54, 2284-2287	5.8	37
361	The roles of buckled geometry and water environment in the excitonic properties of graphitic CN. *Nanoscale*, **2018**, 10, 3738-3743	7.7	14

360	Regulation of Coordination Number over Single Co Sites: Triggering the Efficient Electroreduction of CO. *Angewandte Chemie - International Edition*, **2018**, 57, 1944-1948	16.4	607
359	Ambipolar Half-Metallicity in One-Dimensional Metal(II)(1,2,4,5-Benzenetetramine) Coordination Polymers via Carrier Doping. *Journal of Physical Chemistry C*, **2018**, 122, 989-994	3.8	21
358	Regulation of Coordination Number over Single Co Sites: Triggering the Efficient Electroreduction of CO2. *Angewandte Chemie*, **2018**, 130, 1962-1966	3.6	176
357	A new phase of the two-dimensional ReS2 sheet with tunable magnetism. *Journal of Materials Chemistry C*, **2018**, 6, 1248-1254	7.1	21
356	Spatial and thickness dependence of coupling interaction of surface states and influence on transport and optical properties of few-layer BiSe. *Journal of Physics Condensed Matter*, **2018**, 30, 065503	1.8	2
355	Penta-PtN: an ideal two-dimensional material for nanoelectronics. *Nanoscale*, **2018**, 10, 16169-16177	7.7	30
354	A class of Pb-free double perovskite halide semiconductors with intrinsic ferromagnetism, large spin splitting and high Curie temperature. *Materials Horizons*, **2018**, 5, 961-968	14.4	40
353	A Silver Nanocluster Containing Interstitial Sulfur and Unprecedented Chemical Bonds. *Angewandte Chemie - International Edition*, **2018**, 57, 11273-11277	16.4	39
352	Rational Design of Two-dimensional Anode Materials: BS as a Strained Graphene. *Journal of Physical Chemistry Letters*, **2018**, 9, 4852-4856	6.4	25
351	Atomically thin semiconducting penta-PdP2 and PdAs2 with ultrahigh carrier mobility. *Journal of Materials Chemistry C*, **2018**, 6, 9055-9059	7.1	25
350	Hidden Order and Haldane-Like Phase in Molecular Chains Assembled from Conformation-Switchable Molecules. *ACS Nano*, **2018**, 12, 6515-6522	16.7	0
349	Two-dimensional silicon crystals with sizable band gaps and ultrahigh carrier mobility. *Nanoscale*, **2018**, 10, 1265-1271	7.7	18
348	Manipulation of spin and magnetic anisotropy in bilayer magnetic molecular junctions. *Physical Chemistry Chemical Physics*, **2018**, 20, 26396-26404	3.6	10
347	Significantly enhanced magnetoresistance in monolayer WTevia heterojunction engineering: a first-principles study. *Nanoscale*, **2018**, 10, 22231-22236	7.7	4
346	Single Pt atoms supported on oxidized graphene as a promising catalyst for hydrolysis of ammonia borane. *Chinese Journal of Chemical Physics*, **2018**, 31, 641-648	0.9	7
345	Azide Passivation of Black Phosphorus Nanosheets: Covalent Functionalization Affords Ambient Stability Enhancement. *Angewandte Chemie*, **2018**, 131, 1493	3.6	3
344	Intrinsic Quantum Anomalous Hall Effect with In-Plane Magnetization: Searching Rule and Material Prediction. *Physical Review Letters*, **2018**, 121, 246401	7.4	44
343	Visualizing Elementary Reactions of Methanol by Electrons and Holes on TiO2(110) Surface. *Journal of Physical Chemistry C*, **2018**, 122, 28805-28814	3.8	14

342	Kernel Homology in Gold Nanoclusters. *Angewandte Chemie - International Edition*, **2018**, 57, 15450-15454	16.4	20
341	Kernel Homology in Gold Nanoclusters. *Angewandte Chemie*, **2018**, 130, 15676-15680	3.6	6
340	Intrinsic Electric Fields in Two-dimensional Materials Boost the Solar-to-Hydrogen Efficiency for Photocatalytic Water Splitting. *Nano Letters*, **2018**, 18, 6312-6317	11.5	168
339	Tuning Charge Transport in Aromatic-Ring Single-Molecule Junctions via Ionic-Liquid Gating. *Angewandte Chemie*, **2018**, 130, 14222-14227	3.6	18
338	Obtaining Intrinsically Occupied Free-Space Superatom States in an Encapsulated CaN Nanotube. *ACS Omega*, **2018**, 3, 11966-11971	3.9	3
337	Material Design for Photocatalytic Water Splitting from a Theoretical Perspective. *Advanced Materials*, **2018**, 30, e1802106	24	146
336	Electron-phonon interaction in a Ca2N monolayer: Intrinsic mobility of electrene. *Physical Review B*, **2018**, 98,	3.3	11
335	One-Nanometer-Thick PtNiRh Trimetallic Nanowires with Enhanced Oxygen Reduction Electrocatalysis in Acid Media: Integrating Multiple Advantages into One Catalyst. *Journal of the American Chemical Society*, **2018**, 140, 16159-16167	16.4	111
334	Direct Z-Scheme Water Splitting Photocatalyst Based on Two-Dimensional Van Der Waals Heterostructures. *Journal of Physical Chemistry Letters*, **2018**, 9, 5419-5424	6.4	77
333	A Silver Nanocluster Containing Interstitial Sulfur and Unprecedented Chemical Bonds. *Angewandte Chemie*, **2018**, 130, 11443-11447	3.6	20
332	Tuning Charge Transport in Aromatic-Ring Single-Molecule Junctions via Ionic-Liquid Gating. *Angewandte Chemie - International Edition*, **2018**, 57, 14026-14031	16.4	36
331	Two-dimensional transitional metal dihydride crystals with anisotropic and spin-polarized Fermi Dirac cones. *Journal of Materials Chemistry C*, **2018**, 6, 11243-11247	7.1	7
330	Computation-Guided Development of Platinum Alloy Catalyst for Carbon Monoxide Preferential Oxidation. *ACS Catalysis*, **2018**, 8, 5777-5786	13.1	17
329	Electronic, Optical, and Mechanical Properties of Diamond Nanowires Encapsulated in Carbon Nanotubes: A First-Principles View. *Journal of Physical Chemistry C*, **2017**, 121, 3661-3672	3.8	2
328	First-Principles Study of Molecular Clusters Formed by Nitric Acid and Ammonia. *Journal of Physical Chemistry A*, **2017**, 121, 661-668	2.8	9
327	Enhanced selective oxidation of h-BN nanosheet through a substrate-mediated localized charge effect. *Physical Chemistry Chemical Physics*, **2017**, 19, 4435-4439	3.6	9
326	Transport properties of a three-shell icosahedral matryoshka cluster: a first-principles study. *RSC Advances*, **2017**, 7, 12704-12710	3.7	2
325	Understanding of Strain Effects in the Electrochemical Reduction of CO2: Using Pd Nanostructures as an Ideal Platform. *Angewandte Chemie*, **2017**, 129, 3648-3652	3.6	89

324	Understanding of Strain Effects in the Electrochemical Reduction of CO : Using Pd Nanostructures as an Ideal Platform. *Angewandte Chemie - International Edition*, **2017**, 56, 3594-3598	16.4	229
323	A Kinetic Pathway toward High-Density Ordered N Doping of Epitaxial Graphene on Cu(111) Using CNCl Precursors. *Journal of the American Chemical Society*, **2017**, 139, 7196-7202	16.4	12
322	Single- and few-layer BiOI as promising photocatalysts for solar water splitting. *RSC Advances*, **2017**, 7, 24446-24452	3.7	40
321	Low-dimensional half-metallic materials: theoretical simulations and design. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2017**, 7, e1314	7.9	33
320	Room-Temperature Ferromagnetism in Two-Dimensional FeSi Nanosheet with Enhanced Spin-Polarization Ratio. *Nano Letters*, **2017**, 17, 2771-2777	11.5	147
319	Half-Metallicity in One-Dimensional Metal Trihydride Molecular Nanowires. *Journal of the American Chemical Society*, **2017**, 139, 6290-6293	16.4	37
318	Crystal and Solution Photoluminescence of MAg24(SR)18 (M = Ag/Pd/Pt/Au) Nanoclusters and Some Implications for the Photoluminescence Mechanisms. *Journal of Physical Chemistry C*, **2017**, 121, 13848-13853	3.8	96
317	Sub-nanometre control of the coherent interaction between a single molecule and a plasmonic nanocavity. *Nature Communications*, **2017**, 8, 15225	17.4	113
316	Achieving Remarkable Activity and Durability toward Oxygen Reduction Reaction Based on Ultrathin Rh-Doped Pt Nanowires. *Journal of the American Chemical Society*, **2017**, 139, 8152-8159	16.4	210
315	Role of Surface Stress on the Reactivity of Anatase TiO(001). *Journal of Physical Chemistry Letters*, **2017**, 8, 1764-1771	6.4	29
314	Accurate Determination of the Quasiparticle and Scaling Properties Surrounding the Quantum Critical Point of Disordered Three-Dimensional Dirac Semimetals. *Physical Review Letters*, **2017**, 118, 146401	7.4	12
313	More accurate depiction of adsorption energy on transition metals using work function as one additional descriptor. *Physical Chemistry Chemical Physics*, **2017**, 19, 12628-12632	3.6	28
312	Water on silicene: A hydrogen bond-autocatalyzed physisorption□hemisorption□dissociation transition. *Nano Research*, **2017**, 10, 2223-2233	10	14
311	[TiInO(OOCCH)]: a multifunctional hetero-polyoxotitanate nanocluster with high stability and visible photoactivity. *Dalton Transactions*, **2017**, 46, 678-684	4.3	24
310	□Phosphorene: a new allotrope of phosphorene. *Physical Chemistry Chemical Physics*, **2017**, 19, 2402-2408	3.6	53
309	New insights into the stability and structural evolution of some gold nanoclusters. *Nanoscale*, **2017**, 9, 856-861	7.7	14
308	□Phosphorene: a two dimensional material with a highly negative Poisson's ratio. *Nanoscale*, **2017**, 9, 850-855	7.7	105
307	Porous germanene as a highly efficient gas separation membrane. *Nanoscale*, **2017**, 9, 17505-17512	7.7	9

306	Spin switch in iron phthalocyanine on Au(111) surface by hydrogen adsorption. *Journal of Chemical Physics*, **2017**, 147, 134701	3.9	11
305	Highly Efficient Photocatalytic Water Splitting over Edge-Modified Phosphorene Nanoribbons. *Journal of the American Chemical Society*, **2017**, 139, 15429-15436	16.4	176
304	Gold-Doping of Double-Crown Pd Nanoclusters. *Chemistry - A European Journal*, **2017**, 23, 18187-18192	4.8	19
303	Proximity Effect Induced Spin Injection in Phosphorene on Magnetic Insulator. *ACS Applied Materials & Interfaces*, **2017**, 9, 38999-39010	9.5	13
302	Bottom-up precise synthesis of stable platinum dimers on graphene. *Nature Communications*, **2017**, 8, 1070	17.4	306
301	Two-Dimensional Stoichiometric Boron Oxides as a Versatile Platform for Electronic Structure Engineering. *Journal of Physical Chemistry Letters*, **2017**, 8, 4347-4353	6.4	31
300	Gold atom-decorated CoSe2 nanobelts with engineered active sites for enhanced oxygen evolution. *Journal of Materials Chemistry A*, **2017**, 5, 20202-20207	13	42
299	Electrically driven single-photon emission from an isolated single molecule. *Nature Communications* , **2017**, 8, 580	17.4	67
298	The stabilization of the rocksalt structured tantalum nitride. *Journal of Applied Physics*, **2017**, 122, 045102	2.5	7
297	On the shuttling mechanism of a chlorine atom in a chloroaluminum phthalocyanine based molecular switch. *Physical Chemistry Chemical Physics*, **2017**, 19, 22401-22405	3.6	10
296	Atomic-Level Insight into Optimizing the Hydrogen Evolution Pathway over a Co1-N4 Single-Site Photocatalyst. *Angewandte Chemie*, **2017**, 129, 12359-12364	3.6	28
295	Atomic-Level Insight into Optimizing the Hydrogen Evolution Pathway over a Co -N Single-Site Photocatalyst. *Angewandte Chemie - International Edition*, **2017**, 56, 12191-12196	16.4	183
294	Conjugated Microporous Polymer Nanosheets for Overall Water Splitting Using Visible Light. *Advanced Materials*, **2017**, 29, 1702428	24	211
293	Enhanced photoelectrochemical performance of anatase TiO2 for water splitting via surface codoping. *RSC Advances*, **2017**, 7, 39877-39884	3.7	15
292	Stable Heteropolyoxotitanate Nanocluster for Full Solar Spectrum Photocatalytic Hydrogen Evolution. *Journal of Physical Chemistry C*, **2017**, 121, 18326-18332	3.8	13
291	Two-dimensional multilayer M2CO2 (M = Sc, Zr, Hf) as photocatalysts for hydrogen production from water splitting: a first principles study. *Journal of Materials Chemistry A*, **2017**, 5, 24972-24980	13	53
290	Dominant Kinetic Pathways of Graphene Growth in Chemical Vapor Deposition: The Role of Hydrogen. *Journal of Physical Chemistry C*, **2017**, 121, 25949-25955	3.8	47
289	Two-dimensional van der Waals heterojunctions for functional materials and devices. *Journal of Materials Chemistry C*, **2017**, 5, 12289-12297	7.1	97

288	First-principles study of two-dimensional van der Waals heterojunctions. *Computational Materials Science*, **2016**, 112, 518-526	3.2	72
287	Environment-modulated Kondo phenomena in FePc/Au(111) adsorption systems. *Physical Review B*, **2016**, 93,	3.3	32
286	Quantum stability and magic lengths of metal atom wires. *Physical Review B*, **2016**, 93,	3.3	7
285	Two-dimensional van der Waals nanocomposites as Z-scheme type photocatalysts for hydrogen production from overall water splitting. *Journal of Materials Chemistry A*, **2016**, 4, 18892-18898	13	78
284	Three-Dimensional Covalently Linked Allotropic Structures of Phosphorus. *Journal of Physical Chemistry C*, **2016**, 120, 26453-26458	3.8	5
283	Photochemical Copper Coating on 3D Printed Thermoplastics. *Scientific Reports*, **2016**, 6, 31188	4.9	12
282	Bimetal Doping in Nanoclusters: Synergistic or Counteractive?. *Chemistry of Materials*, **2016**, 28, 8240-8247	9.6	74
281	Kondo screening and spin excitation in few-layer CoPc molecular assembly stacking on Pb(111) surface: A DFT+HEOM study. *Journal of Chemical Physics*, **2016**, 145, 154301	3.9	14
280	Systematic Synthesis of Tellurium Nanostructures and Their Optical Properties: From Nanoparticles to Nanorods, Nanowires, and Nanotubes. *ChemNanoMat*, **2016**, 2, 167-170	3.5	47
279	Anatase TiO2 codoping with sulfur and acceptor IIB metals for water splitting. *International Journal of Hydrogen Energy*, **2016**, 41, 13050-13057	6.7	20
278	Double-hole codoped huge-gap semiconductor ZrO2 for visible-light photocatalysis. *Physical Chemistry Chemical Physics*, **2016**, 18, 17517-24	3.6	23
277	Blockage of ultrafast and directional diffusion of Li atoms on phosphorene with intrinsic defects. *Nanoscale*, **2016**, 8, 4001-6	7.7	65
276	Coherent transport through spin-crossover magnet Fe2 complexes. *Nanoscale*, **2016**, 8, 609-16	7.7	33
275	Two-dimensional interlocked pentagonal bilayer ice: how do water molecules form a hydrogen bonding network?. *Physical Chemistry Chemical Physics*, **2016**, 18, 14216-21	3.6	19
274	Edge-Modified Phosphorene Nanoflake Heterojunctions as Highly Efficient Solar Cells. *Nano Letters* , **2016**, 16, 1675-82	11.5	142
273	Distinct molecule adsorption behaviors on warped nanographene C80H30: A theoretical study. *Carbon*, **2016**, 100, 428-434	10.4	16
272	Nano-scale polar-nonpolar oxide heterostructures for photocatalysis. *Nanoscale*, **2016**, 8, 6057-63	7.7	12
271	Effects of interlayer coupling and electric fields on the electronic structures of graphene and MoS2 heterobilayers. *Journal of Materials Chemistry C*, **2016**, 4, 1776-1781	7.1	89

270	In-gap localized states induced by adsorbates on silicene. *Physical Review B*, **2016**, 93,	3.3	1
269	Partially oxidized atomic cobalt layers for carbon dioxide electroreduction to liquid fuel. *Nature*, **2016**, 529, 68-71	50.4	1231
268	Surface Landau levels and spin states in bismuth (111) ultrathin films. *Nature Communications*, **2016** , 7, 10814	17.4	38
267	Structures and magnetism of mono-palladium and mono-platinum doped Au25(PET)18 nanoclusters. *Chemical Communications*, **2016**, 52, 9873-6	5.8	87
266	Rücktitelbild: The Nanoparticle Size Effect in Graphene Cutting: A "Pac-Man" Mechanism (Angew. Chem. 34/2016). *Angewandte Chemie*, **2016**, 128, 10304-10304	3.6	
265	The Nanoparticle Size Effect in Graphene Cutting: A "Pac-Man" Mechanism. *Angewandte Chemie - International Edition*, **2016**, 55, 9918-21	16.4	22
264	The Nanoparticle Size Effect in Graphene Cutting: A "Pac-Man" Mechanism. *Angewandte Chemie*, **2016**, 128, 10072-10075	3.6	7
263	The g-C3 N4 /C2 N Nanocomposite: A g-C3 N4 -Based Water-Splitting Photocatalyst with Enhanced Energy Efficiency. *ChemPhysChem*, **2016**, 17, 2100-4	3.2	91
262	A many-body GW + BSE investigation of electronic and optical properties of C2N. *Applied Physics Letters*, **2016**, 109, 133108	3.4	32
261	Additive and Photochemical Manufacturing of Copper. *Scientific Reports*, **2016**, 6, 39584	4.9	26
260	Visualizing coherent intermolecular dipole-dipole coupling in real space. *Nature*, **2016**, 531, 623-7	50.4	213
259	Mn2C monolayer: a 2D antiferromagnetic metal with high Néel temperature and large spin-orbit coupling. *Nanoscale*, **2016**, 8, 12939-45	7.7	94
258	Single-layer cadmium chalcogenides: promising visible-light driven photocatalysts for water splitting. *Physical Chemistry Chemical Physics*, **2016**, 18, 17029-36	3.6	55
257	In-situ activated polycation as a multifunctional additive for Li-S batteries. *Nano Energy*, **2016**, 26, 43-49	17.1	28
256	First-principles design of spintronics materials. *National Science Review*, **2016**, 3, 365-381	10.8	191
255	Two-Dimensional Phosphorus Porous Polymorphs with Tunable Band Gaps. *Journal of the American Chemical Society*, **2016**, 138, 7091-8	16.4	96
254	Activating Edge Sites on Pd Catalysts for Selective Hydrogenation of Acetylene via Selective Ga2O3 Decoration. *ACS Catalysis*, **2016**, 6, 3700-3707	13.1	72
253	Point defects in lines in single crystalline phosphorene: directional migration and tunable band gaps. *Nanoscale*, **2016**, 8, 17801-17808	7.7	24

252	A First-Principles Study on Electron Donor and Acceptor Molecules Adsorbed on Phosphorene. *Journal of Physical Chemistry C*, **2015**, 119, 2871-2878	3.8	137
251	Effects of stacking order, layer number and external electric field on electronic structures of few-layer C2N-h2D. *Nanoscale*, **2015**, 7, 14062-70	7.7	147
250	Mono-Mercury Doping of Au25 and the HOMO/LUMO Energies Evaluation Employing Differential Pulse Voltammetry. *Journal of the American Chemical Society*, **2015**, 137, 9511-4	16.4	168
249	Distinguishing adjacent molecules on a surface using plasmon-enhanced Raman scattering. *Nature Nanotechnology*, **2015**, 10, 865-9	28.7	202
248	Single layer of MX□(M = Ti, Zr; X = S, Se, Te): a new platform for nano-electronics and optics. *Physical Chemistry Chemical Physics*, **2015**, 17, 18665-9	3.6	93
247	Rational Design of Cathode Structure for High Rate Performance Lithium-Sulfur Batteries. *Nano Letters*, **2015**, 15, 5443-8	11.5	131
246	Nano-scale displacement sensing based on van der Waals interactions. *Nanoscale*, **2015**, 7, 8962-7	7.7	15
245	Theoretical investigation of gold based model catalysts. *Science China Chemistry*, **2015**, 58, 565-573	7.9	11
244	Copper nanocrystal plane effect on stereoselectivity of catalytic deoxygenation of aromatic epoxides. *Journal of the American Chemical Society*, **2015**, 137, 3791-4	16.4	44
243	Tunable Schottky contacts in hybrid graphene□phosphorene nanocomposites. *Journal of Materials Chemistry C*, **2015**, 3, 4756-4761	7.1	104
242	CO2 Capture on h-BN Sheet with High Selectivity Controlled by External Electric Field. *Journal of Physical Chemistry C*, **2015**, 119, 6912-6917	3.8	127
241	Tetrahedral Au17+: A Superatomic Molecule with a Au13 FCC Core. *Journal of Physical Chemistry C*, **2015**, 119, 23274-23278	3.8	21
240	Structural isomerism in gold nanoparticles revealed by X-ray crystallography. [Corrected]. *Nature Communications*, **2015**, 6, 8667	17.4	208
239	Defects in Phosphorene. *Journal of Physical Chemistry C*, **2015**, 119, 20474-20480	3.8	183
238	SP3-Hybridization Feature of Ag4 Superatom in Superatomic Molecules□*Chinese Journal of Chemical Physics*, **2015**, 28, 476-480	0.9	6
237	Mono-cadmium vs Mono-mercury Doping of Au25 Nanoclusters. *Journal of the American Chemical Society*, **2015**, 137, 15350-3	16.4	159
236	Proposal of a general scheme to obtain room-temperature spin polarization in asymmetric antiferromagnetic semiconductors. *Physical Review B*, **2015**, 92,	3.3	15
235	Synthesis and Properties Evolution of a Family of Tiara-like Phenylethanethiolated Palladium Nanoclusters. *Scientific Reports*, **2015**, 5, 16628	4.9	21

234	Stable Metallic 1T-WS2 Nanoribbons Intercalated with Ammonia Ions: The Correlation between Structure and Electrical/Optical Properties. *Advanced Materials*, **2015**, 27, 4837-44	24	151
233	A Density Functional Study of the Nonlinear Optical Properties of Edge-Functionalized Nonplanar Nanographenes. *ChemPhysChem*, **2015**, 16, 2783-2788	3.2	21
232	Theoretical investigation on icosahedral C60(FeCp)12: A hybrid of C60 and ferrocene. *International Journal of Quantum Chemistry*, **2015**, 115, 1621-1628	2.1	1
231	Comparative Study on Electronic Structures of Sc and Ti Contacts with Monolayer and Multilayer MoS2. *ACS Applied Materials & Interfaces*, **2015**, 7, 12981-7	9.5	33
230	Carbon dimers as the dominant feeding species in epitaxial growth and morphological phase transition of graphene on different Cu substrates. *Physical Review Letters*, **2015**, 114, 216102	7.4	61
229	Adding two active silver atoms on Au□nanoparticle. *Nano Letters*, **2015**, 15, 1281-7	11.5	137
228	Electrical control of carriers' spin orientation in the FeVTiSi Heusler alloy. *Journal of Materials Chemistry C*, **2015**, 3, 2563-2567	7.1	24
227	Formation of bilayer clathrate hydrates. *Journal of Materials Chemistry A*, **2015**, 3, 5547-5555	13	13
226	Highly efficient photothermal effect by atomic-thickness confinement in two-dimensional ZrNCl nanosheets. *ACS Nano*, **2015**, 9, 1683-91	16.7	29
225	A theoretical study of single-atom catalysis of CO oxidation using Au embedded 2D h-BN monolayer: a CO-promoted O□activation. *Scientific Reports*, **2014**, 4, 5441	4.9	177
224	Silicene as a highly sensitive molecule sensor for NH3, NO and NO2. *Physical Chemistry Chemical Physics*, **2014**, 16, 6957-62	3.6	173
223	Negative differential resistance devices by using N-doped graphene nanoribbons. *Journal of Chemical Physics*, **2014**, 140, 164703	3.9	23
222	Electronic structure engineering in chemically modified ultrathin ZnO nanofilms via a built-in heterointerface. *RSC Advances*, **2014**, 4, 18718-18723	3.7	7
221	Density Functional Study of Nonlinear Optical Properties of Grossly Warped Nanographene C80H30. *Journal of Physical Chemistry C*, **2014**, 118, 3313-3318	3.8	21
220	Proposed photosynthesis method for producing hydrogen from dissociated water molecules using incident near-infrared light. *Physical Review Letters*, **2014**, 112, 018301	7.4	163
219	Energy level realignment in weakly interacting donor-acceptor binary molecular networks. *ACS Nano*, **2014**, 8, 1699-707	16.7	32
218	Transition metal atom embedded graphene for capturing CO: A first-principles study. *International Journal of Hydrogen Energy*, **2014**, 39, 20190-20196	6.7	49
217	Double aromaticity in transition metal centered double-ring boron clusters M@B2n (M = Ti, Cr, Fe, Ni, Zn; n = 6, 7, 8). *Journal of Chemical Physics*, **2014**, 141, 124301	3.9	23

216	Active hydrogen species on TiO2 for photocatalytic H2 production. *Physical Chemistry Chemical Physics*, **2014**, 16, 7051-7	3.6	49
215	Ir Detectors: Ultrahigh Infrared Photoresponse from Core□Shell Single-Domain-VO2/V2O5 Heterostructure in Nanobeam (Adv. Funct. Mater. 13/2014). *Advanced Functional Materials*, **2014**, 24, 1820-1820	15.6	2
214	Enhanced photocatalytic mechanism for the hybrid g-C3N4/MoS2 nanocomposite. *Journal of Materials Chemistry A*, **2014**, 2, 7960-7966	13	289
213	CrXTe3 (X = Si, Ge) nanosheets: two dimensional intrinsic ferromagnetic semiconductors. *Journal of Materials Chemistry C*, **2014**, 2, 7071	7.1	262
212	Electronic and optical properties of TiO2 nanotubes and arrays: a first-principles study. *Physical Chemistry Chemical Physics*, **2014**, 16, 11519-26	3.6	16
211	Efficient method for fast simulation of scanning tunneling microscopy with a tip effect. *Journal of Physical Chemistry A*, **2014**, 118, 8953-9	2.8	6
210	Superatom-atom super-bonding in metallic clusters: a new look to the mystery of an Au20 pyramid. *Nanoscale*, **2014**, 6, 12440-4	7.7	41
209	Room-temperature half-metallicity in La(Mn,Zn)AsO alloy via element substitutions. *Journal of the American Chemical Society*, **2014**, 136, 5664-9	16.4	73
208	A first-principles study of gas adsorption on germanene. *Physical Chemistry Chemical Physics*, **2014**, 16, 22495-8	3.6	172
207	Highly confined water: two-dimensional ice, amorphous ice, and clathrate hydrates. *Accounts of Chemical Research*, **2014**, 47, 2505-13	24.3	85
206	Transition between direct gap and indirect gap in two dimensional hydrogenated honeycomb Si x Ge1□ alloys. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	5
205	Obtaining two-dimensional electron gas in free space without resorting to electron doping: an electride based design. *Journal of the American Chemical Society*, **2014**, 136, 13313-8	16.4	204
204	First principles study of fluorine substitution on two-dimensional germanane. *Journal of Physics Condensed Matter*, **2014**, 26, 335302	1.8	11
203	Metal-Free Magnetism and Half-Metallicity of Carbon Nitride Nanotubes: A First-Principles Study. *Journal of Physical Chemistry C*, **2014**, 118, 22491-22498	3.8	16
202	Bilayer Graphene Growth via a Penetration Mechanism. *Journal of Physical Chemistry C*, **2014**, 118, 6201-6206	3.8	39
201	Half-metallicity in MnPSe□exfoliated nanosheet with carrier doping. *Journal of the American Chemical Society*, **2014**, 136, 11065-9	16.4	264
200	Band Structure Tuning of TiO2 for Enhanced Photoelectrochemical Water Splitting. *Journal of Physical Chemistry C*, **2014**, 118, 7451-7457	3.8	77
199	AlxC Monolayer Sheets: Two-Dimensional Networks with Planar Tetracoordinate Carbon and Potential Applications as Donor Materials in Solar Cell. *Journal of Physical Chemistry Letters*, **2014**, 5, 2058-65	6.4	76

198	Methanol-Selective Oxidation Pathways on Au Surfaces: A First-Principles Study. *Journal of Physical Chemistry C*, **2014**, 118, 17511-17520	3.8	19
197	Ferroelectric hexagonal and rhombic monolayer ice phases. *Chemical Science*, **2014**, 5, 1757-1764	9.4	79
196	Porous Boron Nitride with Tunable Pore Size. *Journal of Physical Chemistry Letters*, **2014**, 5, 393-8	6.4	66
195	Evidence of van Hove singularities in ordered grain boundaries of graphene. *Physical Review Letters* , **2014**, 112, 226802	7.4	51
194	Nonnuclear nearly free electron conduction channels induced by doping charge in nanotube-molecular sheet composites. *Journal of Physical Chemistry A*, **2014**, 118, 7255-60	2.8	13
193	Electronic structure and aromaticity of large-scale hexagonal graphene nanoflakes. *Journal of Chemical Physics*, **2014**, 141, 214704	3.9	38
192	SiN-SiC nanofilm: A nano-functional ceramic with bipolar magnetic semiconducting character. *Applied Physics Letters*, **2014**, 104, 172403	3.4	22
191	Understanding the Kondo resonance in the d-CoPc/Au(111) adsorption system. *Journal of Chemical Physics*, **2014**, 141, 084713	3.9	30
190	Ultrahigh Infrared Photoresponse from Core–Shell Single-Domain-VO2/V2O5 Heterostructure in Nanobeam. *Advanced Functional Materials*, **2014**, 24, 1821-1830	15.6	66
189	Topological phase transition driven by a spatially periodic potential. *Physical Review B*, **2014**, 90,	3.3	3
188	Band structure engineering of anatase TiO2 by metal-assisted P-O coupling. *Journal of Chemical Physics*, **2014**, 140, 174705	3.9	23
187	STM tip-assisted single molecule chemistry. *Physical Chemistry Chemical Physics*, **2013**, 15, 12428-41	3.6	21
186	Coherent interference in the resonant dissociative electron attachment to carbon monoxide. *Physical Review A*, **2013**, 88,	2.6	13
185	Superatom networks in thiolate-protected gold nanoparticles. *Angewandte Chemie - International Edition*, **2013**, 52, 9035-9	16.4	98
184	Spin-polarized transport properties of Mn@Au6 cluster. *Chemical Physics Letters*, **2013**, 590, 111-115	2.5	2
183	Bipolar magnetic materials for electrical manipulation of spin-polarization orientation. *Physical Chemistry Chemical Physics*, **2013**, 15, 15793-801	3.6	52
182	Unusual Metallic Microporous Boron Nitride Networks. *Journal of Physical Chemistry Letters*, **2013**, 4, 3484-3488	6.4	69
181	Helium separation via porous silicene based ultimate membrane. *Nanoscale*, **2013**, 5, 9062-6	7.7	82

180	A computational infrared spectroscopic study of graphene oxide. *Journal of Chemical Physics*, **2013**, 139, 084704	3.9	6
179	Structural, electronic, and optical properties of hybrid silicene and graphene nanocomposite. *Journal of Chemical Physics*, **2013**, 139, 154704	3.9	79
178	Hydrogenated bilayer wurtzite SiC nanofilms: a two-dimensional bipolar magnetic semiconductor material. *Physical Chemistry Chemical Physics*, **2013**, 15, 497-503	3.6	52
177	Surface and size effects on the charge state of NV center in nanodiamonds. *Computational and Theoretical Chemistry*, **2013**, 1021, 49-53	2	16
176	Organometallic Hexahapto-Functionalized Graphene: Band Gap Engineering with Minute Distortion to the Planar Structure. *Journal of Physical Chemistry C*, **2013**, 117, 22156-22161	3.8	31
175	Porous silicene as a hydrogen purification membrane. *Physical Chemistry Chemical Physics*, **2013**, 15, 5753-7	3.6	110
174	Control of spin in a La(Mn,Zn)AsO alloy by carrier doping. *Journal of Materials Chemistry C*, **2013**, 1, 7197	7.1	16
173	New insight into the electronic shell of Au(38)(SR)(24): a superatomic molecule. *Nanoscale*, **2013**, 5, 1475-8	7.7	108
172	Hydrogen-incorporated TiS2 ultrathin nanosheets with ultrahigh conductivity for stamp-transferrable electrodes. *Journal of the American Chemical Society*, **2013**, 135, 5144-51	16.4	228
171	Nondecaying long range effect of surface decoration on the charge state of NV center in diamond. *Journal of Chemical Physics*, **2013**, 138, 034702	3.9	6
170	Reply to "Comment on 'two-dimensional boron monolayer sheets'". *ACS Nano*, **2013**, 7, 880-1	16.7	10
169	Exploration of Structures of Two-Dimensional Boron-Silicon Compounds with sp(2) Silicon. *Journal of Physical Chemistry Letters*, **2013**, 4, 561-7	6.4	64
168	Structure sensitivity of low-temperature NO decomposition on Au surfaces. *Journal of Catalysis*, **2013**, 304, 112-122	7.3	49
167	Electronic Stability of Phosphine-Protected Au20 Nanocluster: Superatomic Bonding. *Journal of Physical Chemistry C*, **2013**, 117, 13276-13282	3.8	37
166	Electronic and optical properties of graphene and graphitic ZnO nanocomposite structures. *Journal of Chemical Physics*, **2013**, 138, 124706	3.9	82
165	Communication: new insight into electronic shells of metal clusters: analogues of simple molecules. *Journal of Chemical Physics*, **2013**, 138, 141101	3.9	64
164	Role of point defects on the reactivity of reconstructed anatase titanium dioxide (001) surface. *Nature Communications*, **2013**, 4, 2214	17.4	162
163	Semihydrogenated BN sheet: a promising visible-light driven photocatalyst for water splitting. *Scientific Reports*, **2013**, 3, 1858	4.9	109

162	Orbital-selective single molecule rectifier on graphene-covered Ru(0001) surface. *Applied Physics Letters*, **2013**, 102, 163506	3.4	10
161	Diamond as an inert substrate of graphene. *Journal of Chemical Physics*, **2013**, 138, 054701	3.9	38
160	Orientation-sensitive nonlinear growth of graphene: An epitaxial growth mechanism determined by geometry. *Physical Review B*, **2013**, 88,	3.3	8
159	Diffusion and desorption of oxygen atoms on graphene. *Journal of Physics Condensed Matter*, **2013**, 25, 405301	1.8	16
158	Carrier-tunable magnetism of graphene with single-atom vacancy. *Journal of Applied Physics*, **2013**, 113, 213709	2.5	7
157	Superatom Networks in Thiolate-Protected Gold Nanoparticles. *Angewandte Chemie*, **2013**, 125, 9205-9209	3.9	11
156	Transport spin polarization of magnetic C28 molecular junctions. *Chemical Physics Letters*, **2012**, 535, 111-115	2.5	13
155	High-Pressure Phase Favored by a Symmetry-Recognized Nanoconfinement Effect. *Journal of Physical Chemistry Letters*, **2012**, 3, 2154-8	6.4	2
154	Oxygen molecule dissociation on carbon nanostructures with different types of nitrogen doping. *Nanoscale*, **2012**, 4, 1184-9	7.7	195
153	Half-metallicity in organic single porous sheets. *Journal of the American Chemical Society*, **2012**, 134, 5718-21	13.4	87
152	Two-dimensional boron monolayer sheets. *ACS Nano*, **2012**, 6, 7443-53	16.7	548
151	A theoretical study of spin-polarized transport properties of planar four-coordinate Fe complexes. *Chemical Physics Letters*, **2012**, 539-540, 102-106	2.5	22
150	Efficient spin filter based on FeN4 complexes between carbon nanotube electrodes. *Nanotechnology*, **2012**, 23, 255202	3.4	14
149	Bipolar magnetic semiconductors: a new class of spintronics materials. *Nanoscale*, **2012**, 4, 5680-5	7.7	162
148	Graphene Thickness Control via Gas-Phase Dynamics in Chemical Vapor Deposition. *Journal of Physical Chemistry C*, **2012**, 116, 10557-10562	3.8	59
147	Lattice mismatch induced nonlinear growth of graphene. *Journal of the American Chemical Society*, **2012**, 134, 6045-51	16.4	80
146	Diamondization of chemically functionalized graphene and graphene-BN bilayers. *Physical Chemistry Chemical Physics*, **2012**, 14, 8179-84	3.6	48
145	Iron-phthalocyanine molecular junction with high spin filter efficiency and negative differential resistance. *Journal of Chemical Physics*, **2012**, 136, 064707	3.9	51

144	Why the Band Gap of Graphene Is Tunable on Hexagonal Boron Nitride. *Journal of Physical Chemistry C*, **2012**, 116, 3142-3146	3.8	88
143	Observation of photocatalytic dissociation of water on terminal Ti sites of TiO2(110)-1 □1 surface. *Journal of the American Chemical Society*, **2012**, 134, 9978-85	16.4	137
142	Oxidation of a two-dimensional hexagonal boron nitride monolayer: a first-principles study. *Physical Chemistry Chemical Physics*, **2012**, 14, 5545-50	3.6	77
141	Highly entangled K0.5V2O5 superlong nanobelt membranes for flexible nonvolatile memory devices. *Journal of Materials Chemistry*, **2012**, 22, 18214		18
140	. *Journal of Physical Chemistry C*, **2012**, 116, 11336-11342	3.8	150
139	Giant moisture responsiveness of VS2 ultrathin nanosheets for novel touchless positioning interface. *Advanced Materials*, **2012**, 24, 1969-74	24	324
138	First-principles Study of Adsorption and Dissociation of Methanol on the Pt(100) Surface. *Chinese Journal of Chemical Physics*, **2012**, 25, 199-203	0.9	
137	First-principles Study of Geometric and Electronic Structures of Si(111)-□ □-In Surface Reconstruction. *Chinese Journal of Chemical Physics*, **2012**, 25, 403-408	0.9	6
136	Graphdiyne as Hydrogen Purification Membrane. *Chinese Journal of Chemical Physics*, **2012**, 25, 434-440	0.9	21
135	STM studies of single molecules: molecular orbital aspects. *Chemical Communications*, **2011**, 47, 2747-62	5.8	8
134	Nearly Free Electron State in Graphane Nanoribbon Superlattice. *Chinese Journal of Chemical Physics*, **2011**, 24, 22-24	0.9	14
133	Ultrafast Solid-State Transformation Pathway from New-Phased Goethite VOOH to Paramontroseite VO2 to Rutile VO2(R). *Journal of Physical Chemistry C*, **2011**, 115, 791-799	3.8	41
132	Direct hydrothermal synthesis of monoclinic VO2(M) single-domain nanorods on large scale displaying magnetocaloric effect. *Journal of Materials Chemistry*, **2011**, 21, 4509		88
131	Half-Metallicity in Hybrid Graphene/Boron Nitride Nanoribbons with Dihydrogenated Edges. *Journal of Physical Chemistry C*, **2011**, 115, 9442-9450	3.8	94
130	Structure of Graphene Oxide: Thermodynamics versus Kinetics. *Journal of Physical Chemistry C*, **2011**, 115, 11991-11995	3.8	83
129	Low-temperature growth of graphene by chemical vapor deposition using solid and liquid carbon sources. *ACS Nano*, **2011**, 5, 3385-90	16.7	304
128	First-Principles Thermodynamics of Graphene Growth on Cu Surfaces. *Journal of Physical Chemistry C*, **2011**, 115, 17782-17787	3.8	276
127	Hydroxyls-induced oxygen activation on □hert□Au nanoparticles for low-temperature CO oxidation. *Journal of Catalysis*, **2011**, 277, 95-103	7.3	59

126	Metallic few-layered VS2 ultrathin nanosheets: high two-dimensional conductivity for in-plane supercapacitors. *Journal of the American Chemical Society*, **2011**, 133, 17832-8	16.4	886
125	Half-Metallic Dirac Point in B-Edge Hydrogenated BN Nanoribbons. *Journal of Physical Chemistry C*, **2011**, 115, 17252-17254	3.8	35
124	Are Azafullerene Encapsulated Single-Walled Carbon Nanotubes n-Type Semiconductors?. *Journal of Physical Chemistry C*, **2011**, 115, 12760-12762	3.8	11
123	Oxygen Vacancy-Controlled Reactivity of Hydroxyls on an FeO(111) Monolayer Film. *Journal of Physical Chemistry C*, **2011**, 115, 6815-6824	3.8	33
122	Molecular oxygen adsorption behaviors on the rutile TiO2(110)-1□ surface: an in situ study with low-temperature scanning tunneling microscopy. *Journal of the American Chemical Society*, **2011**, 133, 2002-9	16.4	135
121	CO2 dissociation activated through electron attachment on the reduced rutile TiO2(110)-1□ surface. *Physical Review B*, **2011**, 84,	3.3	59
120	Implementation of screened hybrid density functional for periodic systems with numerical atomic orbitals: basis function fitting and integral screening. *Journal of Chemical Physics*, **2011**, 135, 034110	3.9	20
119	Ferrimagnetism in zigzag graphene nanoribbons induced by main-group adatoms. *Applied Physics Letters*, **2010**, 96, 102503	3.4	37
118	Electrical rectification by selective wave-function coupling in small Ag clusters on Si(111)(7□7). *Physical Review B*, **2010**, 81,	3.3	11
117	Shape-Dependent Reducibility of Cuprous Oxide Nanocrystals. *Journal of Physical Chemistry C*, **2010**, 114, 6676-6680	3.8	79
116	Linear scaling electronic structure calculations with numerical atomic basis set. *International Reviews in Physical Chemistry*, **2010**, 29, 665-691	7	15
115	Electronic Structures and Magnetic Properties of GaN Sheets and Nanoribbons. *Journal of Physical Chemistry C*, **2010**, 114, 11390-11394	3.8	99
114	Electronic, Magnetic, and Transport Properties of Fe-COT Clusters: A Theoretical Study. *Journal of Physical Chemistry C*, **2010**, 114, 11946-11950	3.8	21
113	Important Structural Factors Controlling the Conductance of DNA Pairs in Molecular Junctions. *Journal of Physical Chemistry C*, **2010**, 114, 14240-14242	3.8	10
112	Implementation of exact exchange with numerical atomic orbitals. *Journal of Physical Chemistry A*, **2010**, 114, 1039-43	2.8	16
111	First principles nuclear magnetic resonance signatures of graphene oxide. *Journal of Chemical Physics*, **2010**, 133, 034502	3.9	45
110	Single-molecule chemistry of metal phthalocyanine on noble metal surfaces. *Accounts of Chemical Research*, **2010**, 43, 954-62	24.3	98
109	Communication: Coalescence of carbon atoms on Cu (111) surface: Emergence of a stable bridging-metal structure motif. *Journal of Chemical Physics*, **2010**, 133, 071101	3.9	67

108	Structure dependent quantum confinement effect in hydrogen-terminated nanodiamond clusters. *Journal of Applied Physics*, **2010**, 108, 094303	2.5	20
107	Understanding the concept of randomness in inelastic electron tunneling excitations. *Physical Chemistry Chemical Physics*, **2010**, 12, 12012-23	3.6	11
106	Icosahedral B12-containing core-shell structures of B80. *Chemical Communications*, **2010**, 46, 3878-80	5.8	82
105	Nearly free electron superatom states of carbon and boron nitride nanotubes. *Nano Letters*, **2010**, 10, 4830-8	11.5	39
104	Site-specific photocatalytic splitting of methanol on TiO2(110). *Chemical Science*, **2010**, 1, 575	9.4	143
103	Room-Temperature Ferromagnetic Silver Vanadium Oxide (Ag1.2V3O8): A Magnetic Semiconductor Nanoring Structure. *Advanced Functional Materials*, **2010**, 20, 3666-3672	15.6	30
102	Controlling electronic States and transport properties at the level of single molecules. *Advanced Materials*, **2010**, 22, 1967-71	24	19
101	The Electronic State and Spatial Distribution of Excess Charge Created by Oxygen Vacancies on Titanium Dioxide Surfaces. *Hyomen Kagaku*, **2010**, 31, 474-479		
100	Origin of the Ising ferrimagnetism and spin-charge coupling in LuFe2O4. *Physical Review B*, **2009**, 80,	3.3	27
99	Theoretical study of the molecular and electronic structure of methanol on a TiO2(110) surface. *Physical Review B*, **2009**, 80,	3.3	84
98	Magnetism of semiconductor-based magnetic tunnel junctions under electric field from first principles. *Applied Physics Letters*, **2009**, 94, 252102	3.4	2
97	Design and control of electron transport properties of single molecules. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 15259-63	11.5	74
96	First Principles Study on FeAs Single Layers. *Chinese Journal of Chemical Physics*, **2009**, 22, 139-142	0.9	1
95	Funnel hopping: Searching the cluster potential energy surface over the funnels. *Journal of Chemical Physics*, **2009**, 130, 214112	3.9	50
94	Efficient organometallic spin filter based on Europium-cyclooctatetraene wire. *Journal of Chemical Physics*, **2009**, 131, 104704	3.9	40
93	Density functional study on mechanism of CO oxidation with activated water on O/Au (111) surface. *Science Bulletin*, **2009**, 54, 1973-1977	10.6	6
92	Chiral selective tunneling induced graphene nanoribbon switch. *Frontiers of Physics in China*, **2009**, 4, 373-377		1
91	Exploring at nanoscale from first principles. *Frontiers of Physics in China*, **2009**, 4, 256-268		

90	Band-gap scaling of graphene nanohole superlattices. *Physical Review B*, **2009**, 80,	3.3	115
89	Thermal stabilities of the microhydrated zwitterionic glycine: a kinetics and dynamics study. *Journal of Physical Chemistry A*, **2009**, 113, 480-3	2.8	17
88	What are the adsorption sites for CO on the reduced TiO2(110)-1 x 1 surface?. *Journal of the American Chemical Society*, **2009**, 131, 7958-9	16.4	81
87	Graphene nanoribbon as a negative differential resistance device. *Applied Physics Letters*, **2009**, 94, 173110	3.4	204
86	Magnetic states of zigzag graphene nanoribbons from first principles. *Applied Physics Letters*, **2009**, 94, 223105	3.4	37
85	"Narrow" graphene nanoribbons made easier by partial hydrogenation. *Nano Letters*, **2009**, 9, 4025-30	11.5	115
84	First Principles Study on the Geometric and Electronic Structures of the FeO/Pt(111) Surface. *Journal of Physical Chemistry C*, **2009**, 113, 8302-8305	3.8	33
83	Electronic Structure Engineering via On-Plane Chemical Functionalization: A Comparison Study on Two-Dimensional Polysilane and Graphane. *Journal of Physical Chemistry C*, **2009**, 113, 16741-16746	3.8	122
82	How graphene is cut upon oxidation?. *Journal of the American Chemical Society*, **2009**, 131, 6320-1	16.4	289
81	Oxidation states of graphene: insights from computational spectroscopy. *Journal of Chemical Physics*, **2009**, 131, 244505	3.9	84
80	The electronic structure of oxygen atom vacancy and hydroxyl impurity defects on titanium dioxide (110) surface. *Journal of Chemical Physics*, **2009**, 130, 124502	3.9	183
79	Mechanism for tautomerization induced conductance switching of naphthalocyanin molecule. *Applied Physics Letters*, **2009**, 95, 182103	3.4	21
78	Electronic and Magnetic Properties of Metal Phthalocyanines on Au(111) Surface: A First-Principles Study. *Journal of Physical Chemistry C*, **2008**, 112, 13650-13655	3.8	75
77	A first-principles study of NO adsorption and oxidation on Au(111) surface. *Journal of Chemical Physics*, **2008**, 129, 134708	3.9	46
76	Half-metallicity in edge-modified zigzag graphene nanoribbons. *Journal of the American Chemical Society*, **2008**, 130, 4224-5	16.4	587
75	Half-metallicity in hybrid BCN nanoribbons. *Journal of Chemical Physics*, **2008**, 129, 084712	3.9	129
74	Electronic structures of SiC nanoribbons. *Journal of Chemical Physics*, **2008**, 129, 174114	3.9	199
73	Strain effect on electronic structures of graphene nanoribbons: A first-principles study. *Journal of Chemical Physics*, **2008**, 129, 074704	3.9	157

72	Electronic Structures of Defective Boron Nitride Nanotubes under Transverse Electric Fields. *Journal of Physical Chemistry C*, **2008**, 112, 8424-8428	3.8	28
71	MAGNETISM IN GRAPHENE SYSTEMS. *Nano*, **2008**, 03, 433-442	1.1	61
70	Detecting a Molecule–Surface Hybrid State by an Fe-Coated Tip with a Non-s-Like Orbital. *Journal of Physical Chemistry C*, **2008**, 112, 15603-15606	3.8	14
69	Average density of states in disordered graphene systems. *Physical Review B*, **2008**, 77,	3.3	43
68	POLARIZABILITY AND SHIELDING OF COAXIAL HYBRID DOUBLE-WALLED NANOTUBES: A FIRST-PRINCIPLES STUDY. *Journal of Theoretical and Computational Chemistry*, **2008**, 07, 793-803	1.8	1
67	A first principles study on organic molecule encapsulated boron nitride nanotubes. *Journal of Chemical Physics*, **2008**, 128, 164701	3.9	22
66	Electronic structures of organic molecule encapsulated BN nanotubes under transverse electric field. *Journal of Chemical Physics*, **2008**, 129, 024710	3.9	14
65	Formation and diffusion of oxygen-vacancy pairs on TiO2(110)-(1x1). *Journal of Chemical Physics*, **2008**, 129, 044703	3.9	49
64	Kondo effect in single cobalt phthalocyanine molecules adsorbed on Au(111) monoatomic steps. *Journal of Chemical Physics*, **2008**, 128, 234705	3.9	40
63	Chiral selective tunneling induced negative differential resistance in zigzag graphene nanoribbon: A theoretical study. *Applied Physics Letters*, **2008**, 92, 133114	3.4	81
62	Protonation effects on electron transport through diblock molecular junctions: A theoretical study. *Science in China Series B: Chemistry*, **2008**, 51, 1159-1165		6
61	Hexagonal Cu2SnS3 with metallic character: Another category of conducting sulfides. *Applied Physics Letters*, **2007**, 91, 143104	3.4	77
60	Effects Due to Interadsorbate Interactions on the Dipeptide/TiO2Surface Binding Mechanism Investigated by Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2007**, 111, 7765-7771	3.8	34
59	Mechanism for negative differential resistance in molecular electronic devices: local orbital symmetry matching. *Physical Review Letters*, **2007**, 99, 146803	7.4	135
58	Electronic structure of bilayer graphene: A real-space Green's function study. *Physical Review B*, **2007**, 75,	3.3	32
57	Will zigzag graphene nanoribbon turn to half metal under electric field?. *Applied Physics Letters*, **2007**, 91, 243116	3.4	285
56	Electronic structure of atomic Ti chains on semiconducting graphene nanoribbons: a first-principles study. *Journal of Chemical Physics*, **2007**, 127, 164706	3.9	30
55	Quantum Dot Based on Z-shaped Graphene Nanoribbon: First-principles Study. *Chinese Journal of Chemical Physics*, **2007**, 20, 489-494	0.9	7

54	Linear scaling calculation of band edge states and doped semiconductors. *Journal of Chemical Physics*, **2007**, 126, 244707	3.9	12
53	Geometric and electronic structure of a C60 monolayer on Ag(100). *Physical Review B*, **2007**, 75,	3.3	39
52	Electron-induced ferromagnetic ordering of Co-doped ZnO. *Journal of Applied Physics*, **2007**, 102, 033915	2.5	39
51	Atomic and Molecular Chemisorption of Oxygen in WO4 Clusters. *Chinese Journal of Chemical Physics*, **2007**, 20, 78-82	0.9	6
50	Global minimum structures of morse clusters as a function of the range of the potential: 81. *Journal of Physical Chemistry A*, **2007**, 111, 5287-93	2.8	37
49	Ab initio photoionization dynamics of beta-alanine. *Journal of Chemical Physics*, **2007**, 126, 141103	3.9	12
48	Modified Morse potential for unification of the pair interactions. *Journal of Chemical Physics*, **2007**, 127, 124104	3.9	21
47	Synthesis, Growth Mechanism, and Work Function at Highly Oriented {001} Surfaces of Bismuth Sulfide Microbelts. *Journal of Physical Chemistry C*, **2007**, 111, 12145-12148	3.8	28
46	Bamboolike carbon nitride nanotubes (C9N5H3): Atomic-scale construction, synthesis and lithium battery applications. *Applied Physics Letters*, **2007**, 90, 113116	3.4	8
45	The B3LYP hybrid density functional study on solids. *Frontiers of Physics in China*, **2006**, 1, 339-343		8
44	Geometric and Electronic Properties of Metallofullerene Fe@C60 *Chinese Journal of Chemistry*, **2006**, 24, 1133-1136	4.9	24
43	Linear scaling calculation of maximally localized Wannier functions with atomic basis set. *Journal of Chemical Physics*, **2006**, 124, 234108	3.9	11
42	Linear-scaling density matrix perturbation treatment of electric fields in solids. *Physical Review Letters*, **2006**, 97, 266402	7.4	16
41	Theoretical Study on Geometrical and Electronic Properties of Anionic and Neutral V2O6 Clusters. *Chinese Journal of Chemical Physics*, **2006**, 19, 391-394	0.9	7
40	Structural and electronic properties of OsB2: A hard metallic material. *Physical Review B*, **2006**, 74,	3.3	62
39	CHARGE AND SPIN ORDERING IN Na0.5CoO2 FROM THE HYBRID DENSITY FUNCTIONAL STUDY. *Journal of Theoretical and Computational Chemistry*, **2006**, 05, 515-522	1.8	
38	Ultrafast interfacial proton-coupled electron transfer. *Science*, **2006**, 311, 1436-40	33.3	185
37	Interplay between hydrogen bonding and electron solvation on hydrated TiO2(110). *Physical Review B*, **2006**, 73,	3.3	46

36	One-dimensional transition metal-benzene sandwich polymers: possible ideal conductors for spin transport. *Journal of the American Chemical Society*, **2006**, 128, 2310-4	16.4	185
35	Electronic and magnetic properties of V-doped anatase TiO2 from first principles. *Physical Review B* , **2006**, 74,	3.3	78
34	AFM study of crystalline cellulose in the cell walls of straw. *Polymer International*, **2006**, 55, 87-92	3.3	5
33	Controllable p and n doping of single-walled carbon nanotubes by encapsulation of organic molecules and fullerene: A theoretical investigation. *Applied Physics Letters*, **2005**, 86, 223113	3.4	17
32	Density functional calculations of the polarizability and second-order hyperpolarizability of C50Cl10. *Physical Review A*, **2005**, 71,	2.6	37
31	Wet electrons at the H2O/TiO2(110) surface. *Science*, **2005**, 308, 1154-8	33.3	214
30	Spin-unrestricted linear-scaling electronic structure theory and its application to magnetic carbon-doped boron nitride nanotubes. *Journal of Chemical Physics*, **2005**, 123, 124105	3.9	25
29	Density functional theory study of Wn (n=2) clusters. *Computational and Theoretical Chemistry*, **2005**, 757, 113-118		27
28	Controlling the Kondo effect of an adsorbed magnetic ion through its chemical bonding. *Science*, **2005**, 309, 1542-4	33.3	543
27	Electronic transport properties of Pd-H junctions between two PdHx (x=0,0.25,0.5,0.75,1) electrodes: A nonequilibrium Green function study. *Physical Review B*, **2005**, 72,	3.3	12
26	DENSITY FUNCTIONAL THEORY STUDY OF W5 CLUSTERS. *International Journal of Modern Physics B*, **2005**, 19, 2427-2432	1.1	8
25	Electronic transport in Z-junction carbon nanotubes. *Journal of Chemical Physics*, **2004**, 120, 7733-7	3.9	17
24	A theoretical study of small copper oxide clusters: Cu2Ox (x = 1 - 4). *Journal of Chemical Physics*, **2004**, 120, 2746-51	3.9	25
23	A theoretical study of the Y(mathsf{_{3}})O clusters. *European Physical Journal D*, **2004**, 29, 27-31	1.3	10
22	Fabrication of conjugated polymer arrays by spinodal dewetting. *Polymer International*, **2004**, 53, 1968-1972	3.3	1
21	Is mayenite without clathrated oxygen an inorganic electride?. *Angewandte Chemie - International Edition*, **2004**, 43, 6479-82	16.4	63
20	High-resolution scanning tunneling microscopy for molecules. *Ultramicroscopy*, **2004**, 98, 317-34	3.1	12
19	Deformation-induced site selectivity for hydrogen adsorption on boron nitride nanotubes. *Physical Review B*, **2004**, 69,	3.3	68

18	Hydrogen adsorption on zigzag (8,0) boron nitride nanotubes. *Journal of Chemical Physics*, **2004**, 121, 8481-5	3.9	87
17	Inorganic electride: theoretical study on structural and electronic properties. *Journal of the American Chemical Society*, **2003**, 125, 6050-1	16.4	35
16	Theoretical study of small two-dimensional gold clusters. *Physical Review B*, **2003**, 67,	3.3	106
15	Effects of discrete energy levels on single-electron tunneling in coupled metal particles. *Applied Physics Letters*, **2003**, 82, 3767-3769	3.4	27
14	A theoretical study of the NiO2 species. *Journal of Chemical Physics*, **2003**, 118, 6868-6873	3.9	13
13	Excited states of the 3d transition metal monoxides. *Journal of Chemical Physics*, **2003**, 118, 9608-9613	3.9	54
12	A first-principles study of acetylene and its evolution products on Cu(001). *Journal of Chemical Physics*, **2002**, 116, 3104-3108	3.9	8
11	What can a scanning tunneling microscope image do for the insulating alkanethiol molecules on Au(111) substrates?. *Journal of Chemical Physics*, **2002**, 117, 851-856	3.9	56
10	Nonclassical behavior in the capacitance of a nanojunction. *Physical Review Letters*, **2001**, 86, 5321-4	7.4	68
9	Calculated polarizabilities of small Si clusters. *Physical Review A*, **2000**, 61,	2.6	43
8	Formation energies of topological defects in carbon nanotubes. *Physical Review B*, **2000**, 62, 12652-12655	3.3	59
7	A theoretical study of the CuO3 species. *Journal of Chemical Physics*, **2000**, 113, 7867-7873	3.9	18
6	Theoretical studies of neutral and cationic selenium clusters. *Physical Review B*, **2000**, 62, 17026-17030	3.3	19
5	Negative differential-resistance device involving two C60 molecules. *Applied Physics Letters*, **2000**, 77, 3595-3597	3.4	125
4	A theoretical study of the linear OCuO species. *Journal of Chemical Physics*, **1999**, 111, 1477-1482	3.9	18
3	A New Variational Method for the Coupling System of Polaron in a Quantum Well. *Physica Status Solidi (B): Basic Research*, **1999**, 212, 271-279	1.3	2
2	Nitrogen-inserted nickel nanosheets with controlled orbital hybridization and strain fields for boosted hydrogen oxidation in alkaline electrolytes. *Energy and Environmental Science*,	35.4	4
1	Insights into the effect of substrate adsorption behavior over heme-like Fe1/AC single-atom catalyst. *Nano Research*,1	10	2